Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims

1. (currently amended): A method for selecting at least one lead-candidate compound capable of binding as a ligand to a biopolymer[[,]] from a compound database ~~wherein the lead-candidate compound is a candidate for use as a physiologically active compound when the compound interacts specifically with the biopolymer, comprising:~~

~~obtaining a compound database~~ comprising information on atomic types and covalent bonds of compounds in the database, ~~selecting at least one query molecule capable of binding to the biopolymer, and~~ comprising selecting at least one trial compound by matching ~~the~~ at least one query molecule capable of binding to the biopolymer with trial compounds stored in the database ~~based on information on atomic types and covalent bonds of the at least one query molecule~~ for the mode of covalent bond.

2. (currently amended): The method of claim 1, further comprising ~~modifying~~ constructing the structure of the at least one query molecule by an automatic structure construction method.

3. (previously presented): The method of claim 1, wherein the matching of the at least one query molecule is performed by judging similarity of partial structures based on two-dimensional graphs where each atom is represented as a node and each covalent bond is represented as an arc.

4. (currently amended): The method of claim 3 wherein the matching of the at least one query molecule is performed by ~~the algorithm of Ullman~~ determining correspondence of two dimensional graphs for the query molecule and the trial compound.

5. (currently amended): The method of claim 3 further comprising screening the trial compounds based on information on marker sites in the at least one query molecule[[s]].

6. (currently amended): The method of claim 1, further comprising:

estimating binding schemes of the trial compounds to the biopolymer based on the binding schemes of the at least one query molecule to the biopolymer;

calculating at least one parameter relating to interaction between the trial compounds and the biopolymer; and

screening the trial compounds based on the parameters.

7. (previously presented): The method of claim 1, further comprising:

estimating a virtual receptor model which represents physicochemical environment of the ligand binding site of the biopolymer based on information of three-dimensional structures of one or more known ligands capable of binding to the biopolymer;

judging goodness of fit of the trial compounds to the virtual receptor model; and screening the trial compounds based on the goodness of fit.

8. (currently amended): The method of claim 1, further comprising screening the trial compounds based on at least one parameter selected from number of atoms, number of bonds, number of ring structures, number of atoms for each atomic type, and molecular weight.

9. (previously presented) The method of claim 1, further comprising calculating the interaction energy between the at least one trial compound and the biopolymer.

10. (canceled)